1-Methylpyrene

2381-21-7 | DTXSID0025654

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 94.4 days

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

Image not found
1-Methylpyrene
Measured: 33300
Predicted: 94.4

Image not found
11H-Benzo[a]fluorene
Measured: 88900
Predicted: 121

Image not found
Phenanthrene, trimethyl-
Measured: 26200
Predicted: 75.6

Image not found
Benzo(k)fluoranthene
Measured: 726000
Predicted: 325

Image not found
1-Methyl phenanthrene
Measured: 1370
Predicted: 36.9